Mars 2020 Sample Cleanliness Molecular Transport Model

Ira Katz*, Mark S. Anderson, Lauren M. White, Paul A. Boeder, and William A. Hoey Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA, 91107, USA

ABSTRACT

"NASA's Mars 2020 mission ... rover is being designed to seek signs of past life on Mars, collect and store a set of soil and rock samples that could be returned to Earth in the future." The Mars 2020 Project has a top-level requirement that soil and rock samples contain less than 10 ppb Total Organic Carbon (TOC). The approach taken to meet this requirement is to identify and model for each Mars 2020 mission phase the TOC sources, model TOC transport from sources to sample contacting surfaces, and combine them into an end-to-end model that calculates the TOC in each sample during the mission. The calculations show that Mars 2020 can achieve the TOC sample cleanliness requirement because the project has adopted specific TOC mitigations strategies.

Keywords: Mars 2020, organic carbon, contamination

1. INTRODUCTION

Mars 2020 has a Level 1 Requirement of less than 10 ppb Terrestrial Organic Carbon (TOC) and less than 1 part per billion (ppb) of any of a set of special organic compounds known as "tier one" compounds in the returned samples. The ppb estimates assume a 15 g sample. For a 15 g sample, the 10 ppb requirement corresponds to less than 150 ng TOC per sample tube ². This paper describes how we conservatively calculate and bound the TOC accumulation on the sample tube interior and its cap. Since the tube and seal sample contacting surface areas are about 50 cm², the requirement is that the TOC surface density must be less than 3 ng/cm², more than an order of magnitude less than a molecular monolayer.

The approach taken to meet this requirement is, for each M2020 Mission phase, to identify and model the TOC sources in the Adaptive Caching Assembly (ACA) where the tubes and seals are stored. Then we model TOC transport from sources to sample contacting surfaces (tube interior and sealing plug below the knife edge seal location) for each phase of the mission. Finally, we combine the models into an estimate of TOC for the total mission duration.

1.1 M2020 Mission and Sample Handling Hardware

From the NASA Mars 2020 Mission website 1;

The Mars 2020 rover mission is part of NASA's Mars Exploration Program, a long-term effort of robotic exploration of the Red Planet. The Mars 2020 mission addresses high-priority science goals for Mars exploration, including key questions about the potential for life on Mars. The mission takes the next step by not only seeking signs of habitable conditions on Mars in the ancient past, but also searching for signs of past microbial life itself. The Mars 2020 rover introduces a drill that can collect core samples of the most promising rocks and soils and set them aside in a "cache" on the surface of Mars. A future mission could potentially return these samples to Earth. That would help scientists study the samples in laboratories with special room-sized equipment that would be too large to take to Mars

The mission is timed for a launch opportunity in July/August 2020 when Earth and Mars are in good positions relative to each other for landing on Mars. That is, it takes less power to travel to Mars at this time, compared to other times when Earth and Mars are in different positions in their orbits. To keep mission costs and risks as low as possible, the Mars 2020 design is based on NASA's successful Mars Science Laboratory mission architecture, including its Curiosity rover and proven landing system

Figure 1 shows a CAD drawing of the Mars 2020 rover.

*ira.katz@jpl.nasa.gov



Figure 1. The Mars 2020 rover is based on the Mars Science Laboratory mission's Curiosity rover.

The phases of the M2020 mission² are shown in Figure 2. In this paper, we discuss contamination in the highlighted four boxes: Assembly, Test, and Launch Operations (ATLO); Cruise; Commissioning; and Surface Operations, the mission phases where contamination is most probable.

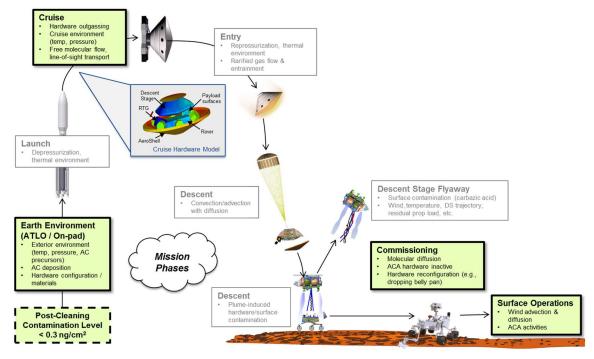


Figure 2. Mars 2020 End-to-End Mission Phases.

M2020 will collect rock cores and regolith samples for return to Earth in Sample Tubes shown in Figure 3. The upper figure is of an empty Sample Tube; the lower figure shows a notional sample inside a sealed tube. The internal surfaces of the titanium (Ti-Al-4V) Sample Tubes are titanium nitride (TiN).

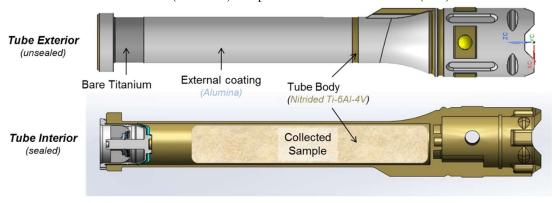


Figure 3. M2020 Sample Tube.

The sample tubes will be stored in protective "gloves" called Fluid Mechanical Particle Barriers³ (FMPBs) as shown in Figure 4. The internal surfaces of the FMPBs are also TiN.

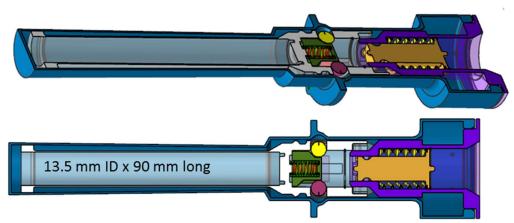


Figure 4. A sheath called a Fluid Mechanical Particle Barrier (FMPB), protects the sample tubes.

As show in Figure 5, the Sample Tubes inside their FMPBs are stored in the Adaptive Caching Assembly (ACA), a box like enclosure located at the front of the Mars 2020 Rover². The ACA dimensions are approximately 0.4m x 0.4m x 0.9m. After commissioning on Mars, the belly pan on the bottom of the ACA will be dropped and the interior exposed to the Mars atmosphere.

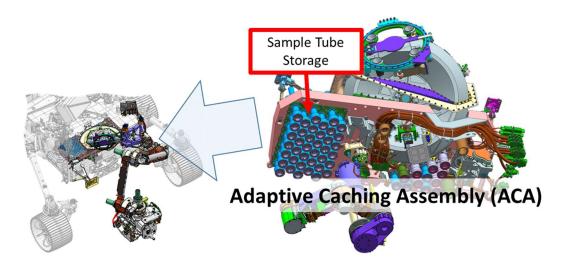


Figure 5. Sample tubes are stored in the Adaptive Caching Assembly (ACA) located in the front of the Rover

1.2 Molecular Contamination Sources

Prior to assembly in the rover during ATLO, the sample tubes and seals are first *pre-cleaned* to a stringent level of less than 100 ng/cm² using conventional aerospace cleaning. This hardware, already very clean by aerospace standards, will then be fired in air at 350°C to remove any remaining organic compounds. After the firing, the sample contacting surfaces of the tubes and seals have a surface TOC density of much less than 1 ng/cm², easily below the Level 1 requirement. The samples will be stored in the hermetically sealed chamber used for the firing. *The issue is how to protect sample contacting surfaces from molecular contamination after the sample tube storage is removed from its hermetic container*.

The sample tube storage is installed in the ACA under clean room conditions. The frequent air changes keep the concentration of large organic molecules very low. The contaminant concentration rises rapidly after the belly pan installation that closes up the ACA. From that time, through the rest of the Mars 2020 mission, the dominant source of molecular organic contamination is outgassing from the ACA hardware. The ACA has cables, motors, connectors and other items that outgas high molecular weight organic molecules. All the materials in the ACA were chosen to have very low out gassing rates and all undergo rigorous thermal vacuum processing. However, the Level 1 requirement is so stringent that if the tubes were exposed for even a few hours in the sealed ACA, they would collect a good fraction of a monolayer, and break the requirement.

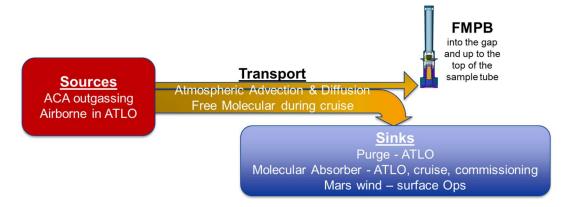


Figure 6. Flux balance between ACA outgassing sources and sinks determines the TOC density near the FMPB gaps.

For most of the mission duration, the sample tubes remain in their protective sleeves, the FMPBs. We calculate the contamination rate in two steps (Figure 6). First, we calculate the TOC concentration in the ACA environment. This requires knowing the outgassing rates inside the ACA, and how those molecules leave the ACA. Second, given a TOC concentration at the base of the FMPBs, we calculate the transport of TOC up the gap between the tube and the sleeve that reach the opening of the sample tube at the top of the FMPB. We including molecular adhesion (gettering) and re-emission from surfaces internal to the FMPBs.

2. MARS 2020 MOLECULAR CONTAMINATION MITIGATION STRATEGY

Testing at JPL showed that uncoated titanium tubes would collect ~ 100 ng/cm² of TOC from the atmosphere. The TOC in a titanium sample tube, $50 \text{ cm}^2 \times 100 \text{ ng/cm}^2$, would be about 5000 ng. That is 30 times the requirement. The result is that the M2020 can only satisfy the Level 1 Requirement because the project has adopted the following four specific mitigation strategies:

- 1. Titanium Nitride (TiN) is used to coat all sample contacting surfaces. TiN provides an inert surface with reduced accumulation of organic contamination. TiN inhibits the chemical absorption of reactive, low molecular weight molecules. The higher molecular weight (MW) organic molecules are limited due to their very low concentration.
- 2. Protect the interiors of the Sample Tubes and the Seals from ambient contamination (higher MW molecules) with a protective "glove" called a "Fluid Mechanical Particle Barrier" (FMPB).
- 3. In the Adaptive Caching Assembly (ACA), use only materials with low outgassing rates that have been vacuum baked.
- 4. Minimize the TOC density in the ACA by removing most of the outgassing products with either a dry nitrogen purge, a large area molecular absorber, or the wind on Mars.

There are a large number of organic molecules, called Adventitious Carbon (AC), in the ambient environment. As shown in Figure 7, not only will high molecular weight organic molecules stick to metal surfaces, but light molecules with hydroxyl and other polar groups can chemisorb on metal oxide surfaces, such as titanium or aluminum after exposure to air. JPL has measured AC accumulation on metal surfaces. On a Ti-6Al-4V surface exposed in a clean room, the AC accumulation asymptotes to about 100 ng/cm2 in about a week, a level that fails to meet the Level 1 requirement.

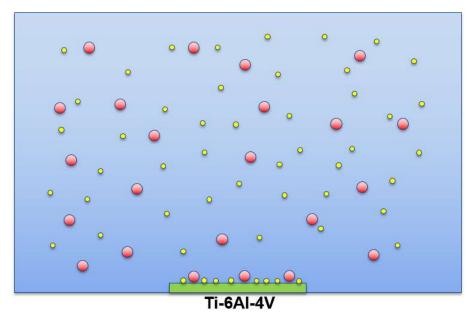


Figure 7. The oxide layer on a Ti-6Al-4V surface can chemisorb light MW organic compounds

To stop light organic molecules from sticking, Professor Francisco Zaera (University of California, Riverside) suggested using a TiN coating. Molecules can only physisorb on surfaces that are chemically inert (e.g. Au or TiN). Since the

residence time is very short for physisorbed low MW molecules, they won't accumulate on such surfaces. However, vapor pressure decreases exponentially with molecular weight; there is a very low concentration of large organic molecules (MW> 200 amu) in the atmosphere. As pictured in Figure 8, this greatly reduces the accumulation of AC on inert surfaces. JPL measurements show that AC accumulation on a TiN surface asymptotes to approximately 40 ng/cm2 after exposure for about a week. If this were the only mitigation, a Sample Tube would launch with about $50 \times 40 = 2000$ ng TOC, still more than six times the requirement

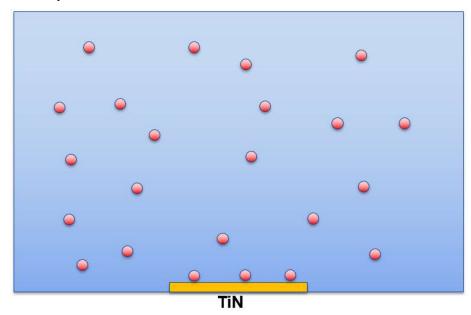


Figure 8. The TiN coating stops light organic molecules from accumulating on surfaces

The second mitigation adopted was to reduce AC accumulation rate using a small opening, a tortuous path, a large area for molecules to adhere before reaching the interior of the sample. The accumulation rate is proportional to molecular flux reaching the interior surface of the sample tube. As shown in Figure 8, the Fluid Mechanical Particle Barrier (FMPB) reduces opening area to less than 1% of the tube interior surface area. The FMPB "glove" provides almost 200 cm² to act as a "getter". As seen in Figure 10, the FMPB concept was inspired by John Canham (Northrop Grumman Innovation System) in 2014. Mikellides, I.G., et al.³ describes how the FMPB protects sample tube interiors from terrestrial biological particles. Below in this paper, we present calculations that show the FMPB is equally effective in stopping organic molecules from contaminating potential samples.

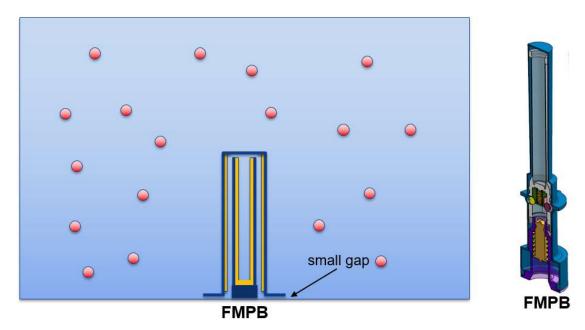


Figure 9. The FMPB reduces the AC accumulation rate with a small opening and a tortuous path

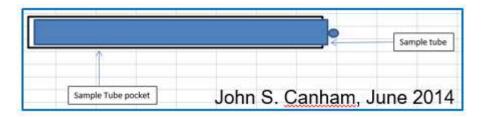


Figure 10. John Canham's original "tube in pocket" concept

The third mitigation is to minimize the outgassing in the ACA. This is accomplished by carefully selecting and using only low outgassing rate materials, and baking them out in vacuum prior to installation in the ACA.

The final mitigation strategy is to reduce the TOC concentration by sweeping outgassing products out of the ACA before they can transport up the FMPBs and into the Sample Tubes. The approach to providing a sink for the outgassing products varies by Mission Phase, as shown in Table 2. For example, during ATLO, ACA outgassing products will be swept out by a dry nitrogen purge right up to launch (see Figure 11)....

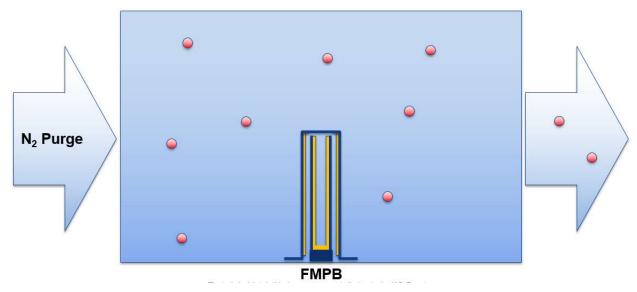


Figure 11. A nitrogen purge will reduce the TOC concentration in ACA right up to launch

Table 1. TOC sinks by Mission Phase.

Mission Phase	TOC Sink
ATLO	N ₂ Purge & Molecular Absorber
Cruise	Molecular Absorber
Commissioning	Molecular Absorber
Surface Operations	Advection & Diffusion

Calculations, described below, show that with these four mitigation strategies, the M2020 approach will meet its Level 1 TOC Requirement using very conservative assumptions.

The analysis approach is, for each mission phase, to calculate the average TOC density, internal to the ACA. We use that average TOC density to find the rate at which TOC molecules are transported into the FMPB, how many stick to the walls and how many make it into the sample tube or onto sample contacting surfaces of the sealing plugs. The area of the gaps at the bottom flange of each FMPB is less than 0.5 cm2, much less than the smallest TOC sink, the Molecular Absorber, whose area is 1000 cm2. Based on the relative areas, we assume that TOC flow into FMPBs does not significantly modify the average TOC density in the ACA.

3. SOURCES: MATERIAL OUTGASSING RATES

Organic materials inside the ACA are the major source of TOC molecules that could contaminate the sample tube. The Mars 2020 project has identified the planned components and estimated material quantities that will contribute to ACA TOC outgassing. We have measured the outgassing rates of the largest known sources following the ASTM E 1559 protocol⁴. At this time, the model uses outgassing rates based on these sample measurements. During ATLO, all the ACA components will be vacuum baked and the direct measurements of the flight unit outgassing will be used in the calculations.

Figure 12 shows an example of the 1559 outgassing data. Rate data from the -100°C QCM is used for the TOC calculations. The change in outgassing rate when the sample temperature increases from 40°C to 70°C in used to determine an Arrhenius energy. The final slope is used as the outgassing rate of the material at 70°C. We don't account for additional decrease of this rate during the duration of the mission.

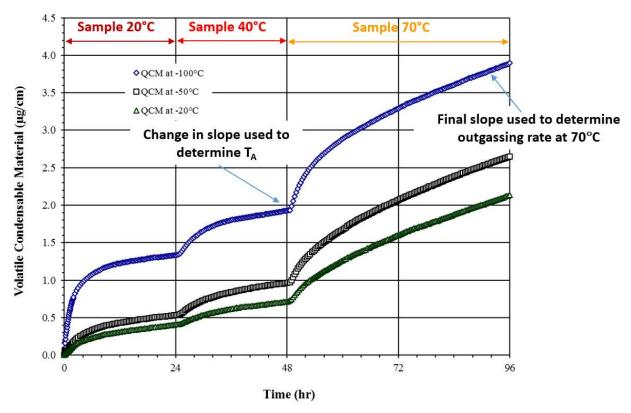


Figure 12. Outgassing data for one of the materials used in the ACA.

The temperature dependence of the outgassing rate is assumed to follow an Arrhenius law.

$$\Gamma(T) = \Gamma_0 \exp\left(-\frac{E_A}{RT}\right)$$

where E_A is the activation energy. For convenience, we express the Activation energy, E_A , in terms of an activation temperature, T_A .

$$\Gamma(T) = \Gamma_0 \exp\left(-\frac{T_A}{T}\right), \quad T_A \equiv \frac{E_A}{R}$$

ACA TOC density, ρ_{TOC} , is determined by balancing the rate that organic molecules are emitted from ACA materials with the rate they are transported out of the ACA volume, as shown in Figure 6. The basic flux balance equation is

4. CALCULATING THE ACA AVERAGE TOC DENSITY

The average ACA TOC density, ρ_{TOC} , is determined by balancing the rate that organic molecules are emitted from ACA materials with the rate they are transported out of the ACA volume (see Figure 6). The basic flux balance equation is

$$\dot{m} = \rho_{TOC} \dot{V}$$

where \dot{m} is the total outgassing rate of materials in the ACA and \dot{V} is a volumetric flow rate. This basic equation, rearranged as

$$\rho_{TOC} = \frac{\dot{m}}{v}.$$
 (2)

is solved for the average TOC density, ρ_{TOC} ,, for all phases of the mission. The only differences are mission phase specific formulations for the volumetric flow rate and ACA temperature.

The transport mechanisms and the TOC sinks for all mission phases are shown in Table 2. In ATLO, outgassing products will be advected out of ACA in a flow of nitrogen gas. In the vacuum of cruise, free molecular flow will transport TOC molecules to a molecular absorber, a 1000 cm2 sheet of Tenax material. During commissioning on Mars, before the ACA belly pan is jettisoned, the outgassed TOC will reach the molecular absorber by atmospheric diffusion. Once the belly pan is gone, TOC products will be swept out of the ACA by the wind on Mars.

Mission Phase	TOC Transport	TOC Sink	
ATLO	Advection/Diffusion	N ₂ Purge & Molecular Absorber	
Cruise	Free Molecular	Molecular Absorber	
Commissioning	Diffusion	Molecular Absorber	
Surface Ops	Advection/Diffusion	Advection & Diffusion	

Table 2. TOC transport mechanisms and sinks for each mission phase.

During purge in ATLO, the volumetric flow rate is just the volumetric flow rate of the purge gas.

$$\dot{V} = \dot{V}_{purge} \tag{3}$$

During cruise, the volumetric flow rate is determined by free molecular flow to the Molecular Absorber.

$$\dot{V} = \frac{\bar{c}}{4} A_{MA} \tag{4}$$

where \bar{c} is the mean molecular speed and A_{MA} is the area of the Molecular Absorbe.

During commissioning on Mars the belly pan remains attached and transport to the Molecular Absorber is by diffusion through the Mars atmosphere inside the ACA.

$$\dot{V} = u_{dif} A_{MA} \tag{5}$$

where u_{dif} is the average diffusion velocity. We approximate the diffusion velocity by

$$u_{dif} \approx \frac{D}{\varrho}$$
 (6)

where D is the diffusion coefficient and ℓ is a characteristic distance the molecules have to travel to reach the molecular absorber, approximately half the depth of the ACA.

$$\ell \approx 0.2 \, m \tag{7}$$

Based on published EPA values, show in Figure 13, we calculate the binary diffusion coefficient, D_{Earth} , on Earth as

$$D_{Ear} = 7.5 \times 10^{-5} \frac{1}{\sqrt{MW}} \frac{m^2}{s}, \tag{8}$$

where MW is the molecular weight of the contaminant molecule.

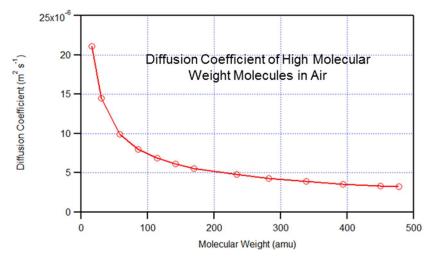


Figure 13. Molecular diffusion coefficients in room temperature air as a function of molecular weight.

When on Mars, the diffusion coefficient increases due to the lower pressure, a factor of about 150. However, this factor is decreased somewhat because the temperatures on Mars are much lower than on Earth, and the molecular weight of the Mars atmosphere, primarily CO₂., is much greater than that of air. In our calculations we assume that the diffusion coefficient on Mars is about 100 times that on Earth.

$$D_{Mars} \approx 100 \times D_{Earth}.$$
 (9)

During Surface Operations on Mars, the ambient wind dominates the volumetric flow rate. The cumulative wind speed distribution measured on Mars by Viking 2⁵ is shown in Figure 13. The average wind speed at a height of 1.6m from the Martian surface.is 4.7 m/s

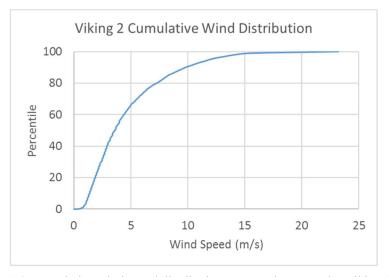


Figure 14. Cumulative wind speed distribution measured on Mars by Viking 2 [9].

To estimate the effective volumetric flow rate for the average Mars wind speed, a 3-D, CFD advection – diffusion calculation was performed using a simplified ACA geometry³. The ACA was modeled as a $0.4 \text{m} \times 0.4 \text{m} \times 0.9$ meter cavity in the body of the rover. The open bottom of the cavity was flush with the belly of the rover and was 0.6 m off the Mars surface. The ACA interior surfaces, were all outgassing at a rate of 1 ng/cm2/hr ($2.8 \times 10^{-12} \text{ kg/m2/s}$). The diffusion coefficient was $7 \times 10^{-4} \text{ m}^2/\text{s}$ and the nominal wind velocity was 4.7 m/s. Figure 14 shows a snapshot of the wind velocity field.

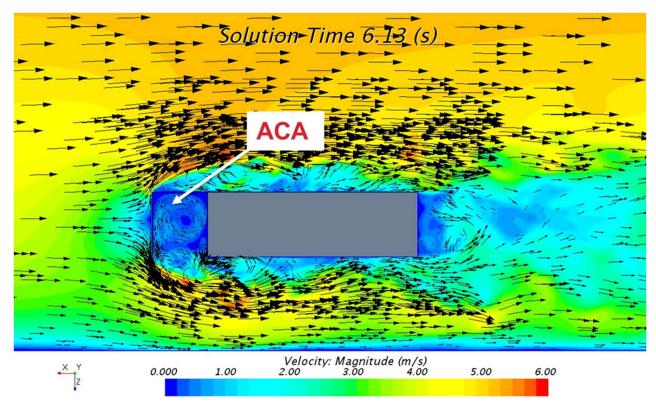


Figure 15. A cross section of the wind velocity field from the 3-D, CFD, advection – diffusion calculation³.

The code output the time averaged TOC molecular density inside the ACA. The mass balance equation was solved for the effective volumetric flow rate given the emission rate and the average TOC density.

$$\dot{V} = u_{eff} A_{MA} \tag{5}$$

The ratio, α_{wind} , between the effective flow velocity and the ambient Mars wind is used to extrapolate to other wind conditions.

$$\alpha_{wind} \equiv \frac{u_{eff}}{u_{wind}} \approx 0.02 \tag{5}$$

5. TOC FLOW PAST THE FMPB

Given the average TOC density in the ACA, we now calculate the rate of TOC flow past the FMPB and into the sample tube. As shown in Figure 16, the FMPB is designed so that TOC must flow through a sequence of long, narrow gaps to get from the ACA into the sample tube. Not only is the path tortuous, but the interior of the FMPB sleeve is also TiN and can collect molecules before they can reach the opening of the sample tube. Calculations presented below show how this "gettering" by the FMPB interior surface effectively protects the tube interior for years on Mars.

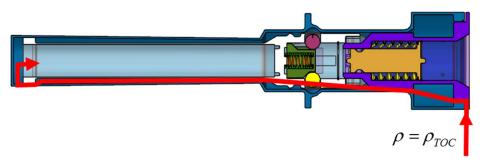


Figure 16. Contaminant molecules must pass through a series of long narrow gasps before reaching the interior of a sample tube.

During ATLO and on Mars, the transport is described by molecular diffusion through the atmosphere and adsorption and desorption from FMB surfaces (gettering). We calculate the amount of TOC that makes it past the FMPB by solving the following couple equations for the TOC density, $\rho(x)$, as a function of distance, x, along the gap, , and the fraction of a monolayer, f(x), condensed on the FMPB walls,

$$\frac{\partial \rho}{\partial t} = D \frac{d^2 \rho}{dx^2} - \frac{\sigma_{max}}{h} \frac{df}{dt}$$
$$\frac{df}{dt} = (1 - f) \frac{\rho \bar{c}}{4\sigma_{max}} - f \frac{1}{\tau_{des}}$$

where σ_{max} is the surface density of a monolayer, \bar{c} is the molecular thermal speed, and τ_{des} is the time for a molecule to desorb from the surface. The second equation describes the effectiveness of the FMPB to act as a getter and trap contamination molecules before they can reach the interior of the sample tube.

Approximate molecular desorption times as function of carbon chain length were obtained from Paserba, K.R. and A.J. Gellman⁶,

$$\tau_{des} = \frac{1}{v_0} exp\left(\frac{E_{des}}{RT}\right), \quad v_0 = 4 \times 10^{19} s^{-1}, \quad E_{des} = -29 + 42\sqrt{n} \frac{kcal}{mol},$$

where n is the number of carbons in the chain. For the conservative estimate, the exact desorption energy as a function of molecular weight is not important, because we find the desorption energy that results in the most contamination and assume all of the outgassing products have that desorption energy.

We solve the two equations numerically by first zoning the length of the FMPB gaps in millimeter increments and time stepping between the diffusion and surface adsorption equations. The diffusion equation is solved implicitly to advance the volume TOC density, ρ . The boundary condition at the opening at the bottom of the FMPB is the average ACA TOC density, ρ_{TOC} , as calculated in the previous section. The second equation advances the surface coverage, f. The surface coverage is assumed to be zero at the start of the calculation. The transport parameters vary with the expected seasonal and diurnal temperature variations during the planned 1000 sol surface operation on Mars. As pointed out above, rather than assume a mixture of molecular weights, we solve this set of equations multiple times, each calculation assuming the contaminants are all alkane chains of a given length with a given E_{des} . We choose the results for the chain length that allows the most contamination into the sample tube to compare with our Level 1 requirement. Since the equations are linear in surface density, it follows than any mixture of molecules will result in less contamination than a sample consisting of only the worst-case molecular weight.

Since the molecular mean free path during cruise is much greater than FMPB channel dimensions, the transport physics can no longer described by molecular diffusion. Rather, a free molecular transport algorithm is used. The MOLFLOW+ code developed by Kersevan et al.⁷ was used to calculate normalized "transmission fractions", the sum of trial molecules sticking onto sensitive surfaces divided by the total number of trial molecules. The calculations were performed using FMPB geometries transferred directly from CAD files. For these calculations, we assumed no gettering by FMPB surfaces, a very conservative assumption (see Figure 17). Even with this assumption the contamination during cruise is very low, primarily because the rover temperature, and therefore the outgassing rate, is low. The predicted cruise temperatures use telemetry from the flight of the Curiosity rover.

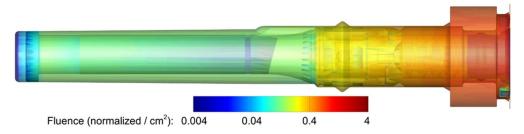


Figure 17. Molecular fluence onto the internal structure of the sample tube and FMPB calculated with a Monte Carlo ray-tracing technique. If all other surfaces diffusely reflect, total transfer to the mouth of the sample tube is less than 0.2% of the mass that enters the gap at the bottom of the FMPB.

6. TOC ESTIMATE FOR THE MARS 2020 MISSION

To obtain an estimate of the maximum contamination in any sample, we have examined every mission phase and examined what processes could allow terrestrial organic molecules to be sealed in within a tube with a Mars sample. While there are several other potential contamination vectors, the processes described in this paper, for the worst case molecular weight distribution, the TOC that diffuses into the sample tube interior and on to the sample contacting surfaces of the sample cap, account for over 75% of the potential contamination. This is not an assumption, but the product of an extensive examination of all the vectors suggested by the molecular contamination team and several external review boards.

Some of the other major sources are accumulation into the tube and onto the cap during the couple of hours that they are not protected by their FMPBs. That is during the sampling process before the sample tube is sealed. Less than 10 ng will accumulated in that time. We have performed CFD calculations of how Rover outgassing may contaminate the surrounding sample sites (J. Rabinovitch and I. Katz⁸). The calculations show that the even in the worst case, the accumulation on the soil would be a tiny contribution to sample contamination. Direct transfer from drill bits to the sample is also small. The cap has very stringent sealing requirements that eliminate the possibility of significant transfer from the Earth's atmosphere during return to Earth. We did a thorough analysis of possible heat shield pyrolysis products during entry, descent and landing, and found that the amount of material ingested by a sample was insignificant.

Table 2 shows our Conservative Estimate for TOC in a sealed sample upon return to Earth. The conservatism in the estimate comes from the following factors:

- 1. During ATLO, the tube storage in the ACA with the belly pan on for 134 days. This assumes 120 days prior to the launch window and a 14 day launch window. Because the temperature (20°C) in the ACA during ATLO is higher than any other time in the mission, the outgassing rate is also higher.
- 2. The TOC is assumed all to have the worst case desorption energy for penetrating past the FMPB. The actual outgassing products will have a range of desorption energies. The coverage of those with lower desorption energies will not stick long enough to coat the FMPB walls; those with higher energies will stick near the entrance to the FMPB and never migrate to in to reach sample contacting surfaces.
- 3. The sample is taken and sealed at the end of the Mars 2020 mission, after 1000 sols on Mars. Most samples will be taken well before the end of the mission when less TOC will have entered the FMPBs.
- 4. The sample cap has been at the bottom of the stack for the entire duration of the mission. Based on free mocular transport calculations, we assume 60% of the TOC that gets past the cap dispenser FMPB lands on sample contacting surfaces of the bottommost of the seven caps. The contamination on that bottom seal accounts for more than half the TOC in the conservative cased. Samples sealed with any of the other six caps will have much less TOC

Even with these conservative assumptions, our calculations show that samples cached by Mars 2020 for potential return to Earth will have TOC contamination levels well below the 10 ppb Level 1 requirement.

Table 3. Estimate of total TOC in a Sample (Conservative Estimate).

Name	Description	TOC (ng)	TOC (ppb)
Tube Interior	While protected by the FMPB	20.5	1.37
Bottom Sample Cap	While protected by the FMPB	51.8	3.45
Open	Accumulation when tube and cap are open on Mars	8.5	0.57
Mars Surface	Accumulation on Mars surface prior to coring (rover outgassing)	3.0	0.20
Coring	Transfer to sample during sample acquisition	5.7	0.38
Volume Probe	Contact transfer from volume probe	0.6	0.04
Post sealing: M2020	Leak rate through seal while carried by M2020	1	0.07
Post sealing: future missions	Future missions leak rate	3	0.20
Total Estimate		94	6.3
Baseline L1 Requirement		150	10
Margin (as % of L1 Baseline)		37%	37%

7. CONCLUSIONS

The Mars 2020 project has a Level 1 requirement to have less than 10 ppb of terrestrial organic carbon in encapsulated samples for return. This requirement is more stringent than previous missions, and will be met because of extraordinary measures taken by Mars 2020 project. When installed in the Mars 2020 rover, the sample tubes have less than 1 ppb TOC. The additional TOC comes from outgassing by the Mars 2020 Rover during the mission. The in the ACA, the section of the Rover where the sample tubes are stored and manipulated, will contribute most of the contaminant molecules. Because most of the accumulation occurs after the rover is sealed up prior to launch and continues for the duration of the mission, verifying that the Level 1 requirement is by analysis; testing alone is not enough. However, the analysis relies measured outgassing rates of Mars 2020 hardware. The Mars 2020 project has performed numerous tests to validate as many components of the analysis model as possible.

Eigenbrode et al.⁹ reported measurements by the Sample Analysis at Mars instrument suite onboard the Curiosity Rover that show significant concentrations of organic carbon containing molecules in martian samples. The reported concentration of these organic molecules was very high compared with the Mars 2020 Level 1 requirement of 10 ppb. This discovery demonstrates the existence of complex organic molecules on Mars and increases the likelihood that should samples cached by Mars 2020 be returned to Earth, they will contain organic molecules of extraterrestrial origin. The TOC contamination control efforts by the Mars 2020 project reported in this paper will ensure that, if the samples are returned from Mars, the signatures from Mars organic molecules, if at the concentrations reported by Eigenbrode et al., will not be masked by contamination of terrestrial origin.

8. ACKNOWLEDGEMENTS

The research described in this paper was carried out by the Jet Propulsion Laboratory, California Institute of Technology, under a contract with the National Aeronautics and Space Administration. The authors would like to thank Professor Francisco Zaera, UC Riverside, for his valuable contributions to this effort, in particular for suggesting the use of TiN surface coatings. We would also like Dr. Genevieve Devaud, Ball Aerospace, for several informative discussions as part of our external review process.

REFERENCES

- [1] https://mars.nasa.gov/mars2020/mission/overview
- [2] Lauren White, et al., "Organic and inorganic contamination control approaches for return sample investigation on Mars 2020", 2017 IEEE Aerospace Conference
- [3] Mikellides, I.G., et al., "The viscous Fluid Mechanical Particle Barrier for the prevention of sample contamination on the Mars 2020 mission", Planetary and Space Science 142 (2017) 53–68
- [4] ASTM E 1559, "Standard Test Method for Contamination Outgassing Characteristics of Spacecraft Materials
- [5] http://www-k12.atmos.washington.edu/k12/resources/mars_data-information/data.html
- [6] Paserba, K.R. and A.J. Gellman, "Kinetics and Energetics of Oligomer Desorption from Surfaces", Phys. Rev. Lett 86, 2001
- [7] Kersevan, R., and Pons, J.-L. "Introduction to MOLFLOW+: New graphical processing unit-based Monte Carlo code for simulating molecular flows and for calculating angular coefficients in the compute unified device architecture environment." *Journal of Vacuum Science and Technology A: Vacuum, Surfaces, and Films* **27**, 1017 (2009).
- [8] J. Rabinovitch and I. Katz, "Surface Deposition of Molecular Contaminants in the Mars 2020 RoverWake", AIAA Aviation Forum 2018 Fluid Dynamics Conference, AIAA 2018-2899
- [9] Eigenbrode et al., "Organic matter preserved in 3-billion-year-old mudstones at Gale crater, Mars", Science 360, 1096–1101 (2018) 8 June 2018